



Ising and anisotropic Heisenberg magnets with mobile defects

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Abstract

Motivated by experiments on $(\text{Sr,Ca,Lu})_{14}\text{Cu}_{24}\text{O}_{41}$, a two-dimensional Ising model with mobile defects and a two-dimensional anisotropic Heisenberg antiferromagnet have been proposed and studied recently. We extend previous investigations by analysing phase diagrams of both models in external fields using mainly Monte Carlo techniques. In the Ising case, the phase transition is due to the thermal instability of defect stripes, in the Heisenberg case additional spin-flop structures play an essential role.

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1. Introduction

The compounds $(\text{Sr,Lu,Ca})_{14}\text{Cu}_{24}\text{O}_{41}$ display interesting low-dimensional magnetic features arising from Cu_2O_3 two-leg ladders and CuO_2 chains. Here, we shall consider two types of models which have been motivated by experimental observations on the CuO_2 chains [1,2,3,4].

On the one hand, a simple two-dimensional Ising model with mobile defects has been introduced [5]. The spins correspond to the magnetic Cu^{2+} ions, and the defects to those Cu ions which are believed to be spinless due to holes (Zhang–Rice singlets). The defects have been shown to form, at low temperatures, nearly straight stripes, perpendicular to the CuO_2 chains. The coherency of the stripes gets lost at a phase transition of first order [5,6].

On the other hand, Matsuda *et al.* [3] proposed a two-dimensional anisotropic Heisenberg model, with an easy spin axis, which reproduced nicely the measured spin-wave dispersions in $\text{La}_5\text{Ca}_9\text{Cu}_{24}\text{O}_{41}$. In subsequent analyses of this model [7,8], the effect of external fields parallel (leading to a spin-flop phase)

and perpendicular to the easy axis on various thermal quantities has been analysed and compared to experimental findings [2,4].

In this contribution, we shall extend the previous work on both models in external fields. For the Ising model with a local pinning potential, the phase diagram in the (temperature, field)–plane is determined at various pinning strengths. In the Heisenberg case, the boundary of the antiferromagnetic phase and the transition to the spin-flop phase are studied in detail, both for the model of Matsuda *et al.* as well as for a simpler, more common variant of the anisotropic Heisenberg antiferromagnet [9].

2. Ising model with mobile defects

The Ising model with mobile defects is defined on a square or rectangular lattice with one axis defining the chain direction (horizontal direction in Fig. 1) [5,6]. Each lattice site is occupied either by a spin, $S_i = \pm 1$, or by a defect, $S_i = 0$. Usually, the concentration of defects is fixed to be ten percent of the lattice sites, as it seems to be the case in $\text{La}_5\text{Ca}_9\text{Cu}_{24}\text{O}_{41}$. Defects are assumed to be mobile along the chains, keeping a minimal distance of two lattice spacings. Neighbouring spins are coupled ferromagnetically, $J > 0$, along the

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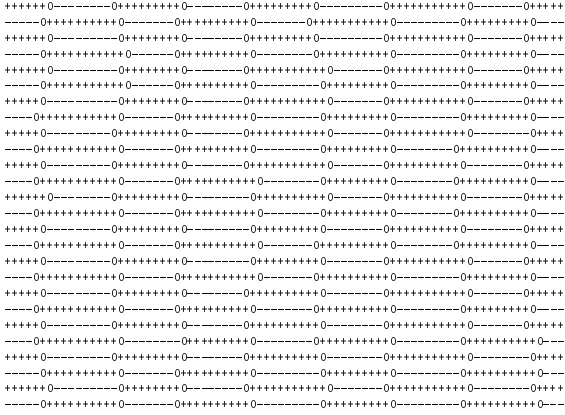


Fig. 1. Typical equilibrium configuration with zig-zag structures in the minimal Ising model, at $k_B T/|J_a| = 0.2$ and $E_p/|J_a| = 0.1$. Only a part of the system with totally 80×80 sites is shown.

chains, and antiferromagnetically, $J_a < 0$ perpendicular to them. In addition, next-nearest neighbouring spins in the same chain separated by a defect interact antiferromagnetically, $J_0 < 0$, as suggested by experiments. Assuming J and J_0 to be large compared to $|J_a|$, one arrives at a ‘minimal version’ of the model, where spins along a chain have the same sign between two defects, reversing sign at a defect. The only relevant energy parameter is J_a [5,6].

The model, in its minimal and full variants, is known to form straight defect stripes, perpendicular to the chains, in the ground state, $T = 0$, with arbitrary separation between the stripes. As temperature T is increased the stripes will meander, tending to keep, on average, their largest possible distance due to entropic repulsion. Eventually the stripes will break up at a phase transition of first order, associated with a pairing of defects. We introduce a local pinning with strength E_p of the defects at the sites of straight equidistant lines perpendicular to the chains. At low temperatures, the stripes stay close to the pinning lines and long-range antiferromagnetic order is observed. The transition remains to be of first order, driven, again, by the enhanced pairing of defects [6].

Applying now an external field H in the Ising direction, the ground state continues to consist of straight stripes at sufficiently low fields. At $H_1 < H < H_2$, assuming a vanishing or weak pinning potential, the defects will form zig-zag stripes separating the antiferromagnetic domains, thereby allowing for a non-zero total magnetization, see Fig. 1 for a typical equilibrium configuration at low temperatures. For $H > H_2$, in the minimal model the defects will be paired, with isolated spins between two neighbouring defects pointing opposite to the field direction. In the full model, even those spins may be reversed in even stronger fields.

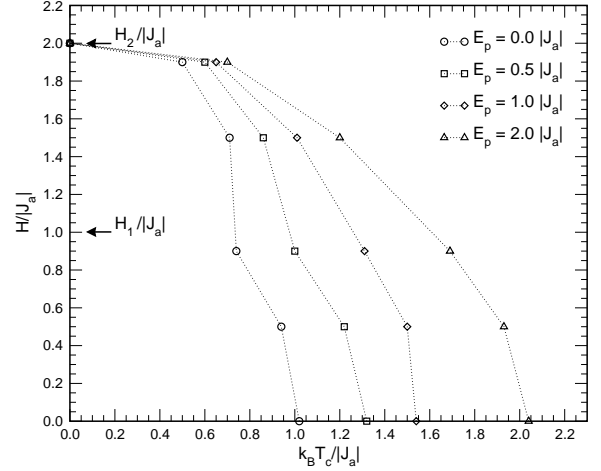


Fig. 2. Phase diagram of the minimal Ising model with various pinning strengths, E_p .

Upon increasing the temperature, at fixed field $H < H_2$, the Ising magnet will undergo a phase transition at which the defect stripes, being either straight or of zig-zag type, become unstable. Indeed, performing extensive Monte Carlo simulations, we determined phase diagrams of the Ising model in the (T, H) -plane, as depicted in Fig. 2 for the minimal variant with different pinning strengths, E_p [10].

In particular, we find no evidence for a transition associated with the zig-zag structure. Albeit there is a jump in the total magnetization, and thence a divergence in the susceptibility, at $T = 0$ and $H = H_1$, these quantities change smoothly even at very low temperatures. Indeed, small zig-zag segments are thermally excited well below H_1 , with a gradual increase of their average length as H is increased [10].

A large pinning potential may suppress the zig-zag structures in the minimal and full models [10].

We conclude that the zig-zag structures are presumably not relevant in explaining the transition from the antiferromagnetic to the disordered phase in $(\text{La,Ca})_{14}\text{Cu}_{24}\text{O}_{41}$ [2,4]. However, a melting of extended or local defect stripes may play an important role in that transition.

3. Anisotropic Heisenberg antiferromagnet

Following Matsuda *et al.* [3], the magnetic properties of $\text{La}_5\text{Ca}_9\text{Cu}_{24}\text{O}_{41}$ depend on the Cu^{2+} ions located in the ac -planes, having a centered rectangular geometry, see Fig. 3. Based on their spin-wave analysis, the spins ($S = 1/2$) of the ions couple along the CuO_2 chains, i.e. along the c axis (vertical direction in Fig. 3), through nearest neighbour, J_{c1} , and next-nearest neighbour, J_{c2} , exchange constants, with $J_{c1} = -0.2$

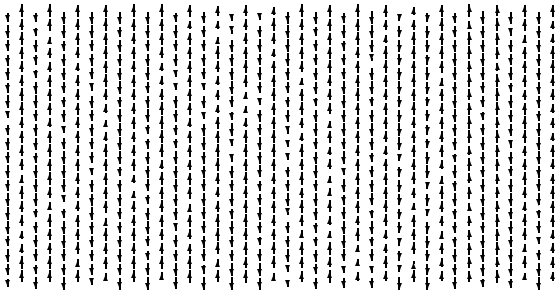


Fig. 3. Typical equilibrium configuration of the z -components of the spins in the antiferromagnetic phase of a classical variant of the anisotropic Heisenberg model of Matsuda *et al.* [3] without field, at $k_B T = 0.5$ meV. Only a part of the system with totally 40×40 sites is shown.

meV being antiferromagnetic and $J_{c2} = 0.18$ meV being ferromagnetic. The ferromagnetic ordering in the chains is due to the strong antiferromagnetic inter-chain couplings: $J_{ac1} = -0.681$ meV refers to the two nearest neighbours in the adjacent chain, and $J_{ac2} = -0.3405$ meV denotes the couplings to the two next-nearest neighbours.

Importantly, there is an uniaxial anisotropy favouring alignment of the spins along the b axis. Its contributions to the different couplings are not known, and its total effect may be mimicked in the classical variant of the model with spins of length one by a single-ion interaction $D = -0.211$ meV.

We studied the classical model with external fields along the easy axis, H_z , and perpendicular to it, H_x , doing Monte Carlo simulations. In both cases, one encounters an antiferromagnetic phase at low fields, see Fig. 3. The complete phase diagrams, as obtained from finite-size analyses of the simulation data, are shown in Fig. 4. In the case of H_x , the phase transition is continuous, being in the Ising universality class. More interestingly, in the case of H_z , there is a spin-flop-phase with algebraically decaying spin correlations. The boundary of the antiferromagnetic phase is, at low fields, in the Ising universality class as well. As suggested by the behaviour of the Binder cumulant, the transition between the antiferromagnetic and paramagnetic phases eventually becomes of first order as the field is increased, with a tricritical point at about $k_B T \approx 0.79$ meV [8]. At even stronger fields, one encounters, closely, at $k_B T \approx 0.75$ meV [8], a triple point between these two and the spin-flop phases.

Our preliminary Monte Carlo study on the standard classical anisotropic Heisenberg model with nearest neighbour antiferromagnetic interactions in two dimensions [9] suggests that the phase diagram keeps the same topology for that simpler model, as had been proposed before for its quantum version [11].

Note that experiments on $\text{La}_5\text{Ca}_9\text{Cu}_{24}\text{O}_{41}$ do not

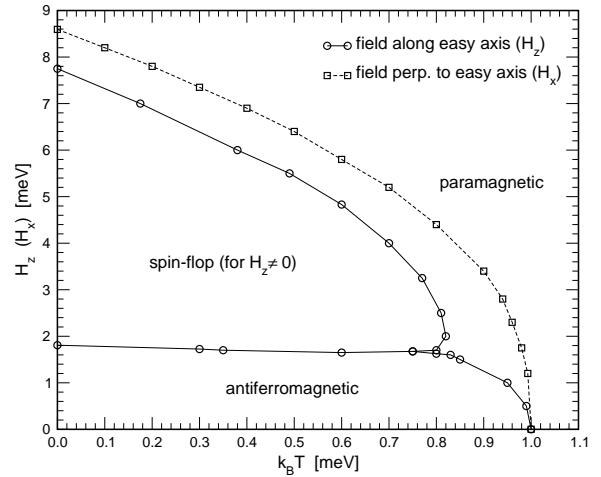


Fig. 4. Phase diagrams of the anisotropic Heisenberg model [3] with fields parallel and perpendicular to the easy axis of the spin couplings.

show a direct transition between the antiferromagnetic and spin-flop phases [2,4,7]. This may be due to defects which have not been taken into account in the model of Matsuda *et al.* Their possible influence has been discussed elsewhere [8].

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